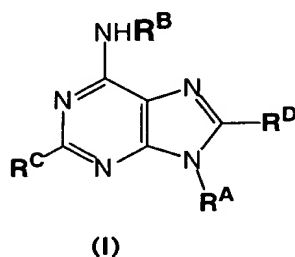


## Claims

1. A compound of formula (I) (or a pharmaceutically acceptable derivative thereof):



wherein

$R^A$  is hydrogen, or an aliphatic, heteroaliphatic, aryl, or heteroaryl moiety;

10  $R^B$  is an aliphatic, heteroaliphatic, aryl, or heteroaryl moiety which comprises one or more phosphorus-containing moieties;

$R^C$  is hydrogen, halogen, an aliphatic, heteroaliphatic, aryl, or heteroaryl moiety, or -ZR, wherein Z is -O-, -S-, or NR, wherein each occurrence of R without a further alphanumeric superscript is independently hydrogen, or a substituted or unsubstituted aliphatic, heteroaliphatic, aryl, or heteroaryl moiety;

15  $R^D$  is hydrogen, halogen, an aliphatic, heteroaliphatic, aryl, or heteroaryl moiety, or -ZR; wherein in each of the foregoing groups each aliphatic or heteroaliphatic moiety may be branched or unbranched, cyclic or acyclic and substituted or unsubstituted, and each aryl and heteroaryl moiety may be substituted or unsubstituted;

with the following provisos:

20 (A) (1)  $R^D$  is a moiety other than one comprising a substituted or unsubstituted arylene moiety (in which up to two methine carbons may be replaced by nitrogen atoms), a C3-7 cycloalkylene moiety (which may contain nitrogen atoms in place of up to two ring carbons), an indanylene moiety, or a 1,2,3,4-tetrahydronaphthylene moiety; or (2)  $R^D$  is a moiety other than one terminating in a cyano group or in an N-substituted or unsubstituted amino, amidino, guanidino or guanidinoalkyl group;

(B) in compounds in which  $R^C$  is H, OH, halogen, alkoxy or cycloalkoxy groups of 1 to 6 carbon atoms (which alkoxy and cycloalkoxy groups can be substituted with phenyl) or amine, which can be substituted with phenyl or with alkyl or cycloalkyl groups of 1 to 6 carbon atoms, and  $R^A$  is benzyl, 30 phenyl or C1-4 alkyl, optionally substituted with oxygen (e.g. in the form of an ether or alcohol),  $R^B$  is a moiety other than a heteroatom- and halogen-substituted derivative of a 3 to 8 carbon cycloalkyl, a 1 to 10 carbon alkyl, a 6 to 13 carbon aryl, or a 7 to 14 carbon aralkyl moiety in which the heteroatom is selected from N, P, S and O; and,

(C) (1) at least one of  $R^A$ ,  $R^C$  or  $R^D$  comprises a phosphorus-containing moiety; (2)  $R^C$  is covalently attached through a C-C bond to the carbon atom at ring position 2 of the purine ring system; or (3)  $R^B$  comprises a phosphorus-containing moiety other than  $-P(O)R^J R^{J'}$  where  $R^J$  and  $R^{J'}$  are independently OH, alkoxy, arylalkoxy, aryloxy, alkylcarbonyloxy-alkoxy, arylalkylcarbonyloxyalkoxy,  $NR^k R^{k'}$ , mono- or di-alkylaminocarbonylmethyloxy, (di-aryl-alkylaminocarbonylmethyloxy, arylamino, a D- or L- amino acid, N-alkyl)piperidine-4yloxy, 2-methylsulfonylethoxy, 1,3 thiazole-2-ylmethyloxy, 3-pyridylmethyloxy, or 2-((di-alkyl)amino)ethoxy, where  $R^k$  is H, alkyl, cycloalkyl, cycloalkylalkyl, or aryl or arylalkyl (1-5 carbon atoms of the aryl ring may be replaced with N, O or S), or  $R^k$  and  $R^{k'}$  together with the atoms that connect them form a ring system (which can also contain additional N, O or S atoms and which can be saturated or unsaturated).

2. The compound of claim 1, wherein the phosphorus-containing moiety in  $R^B$  is an aliphatic, heteroaliphatic, aryl, or heteroaryl group which comprises at least one of the substituents set forth in Series II:



wherein each occurrence of K is independently -O- or -S-;

each occurrence of Y is independently -O-, -S-, -NR- or a chemical bond linking  $R^1$  to P;

each occurrence of R (without a further alphanumeric superscript) is independently hydrogen, or a substituted or unsubstituted aliphatic, heteroaliphatic, aryl, or heteroaryl moiety;

each occurrence of  $R^1$  is independently a substituted or unsubstituted aliphatic, heteroaliphatic, aryl, or heteroaryl moiety, or, except in  $YR^1$  moieties in which Y is a covalent bond,  $R^1$  may also be H;

each occurrence of  $R^2$  is independently  $R^1$ ,  $-PK(YR^1)(YR^1)$ ,  $-SO_2(YR^1)$  or  $-C(O)(YR^1)$

each occurrence of G is independently -O-, -S-, -NR- or  $M_x$ ;

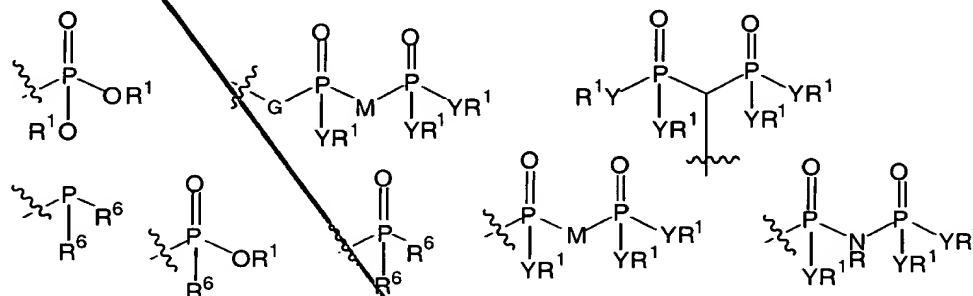
each occurrence of M is independently a substituted or unsubstituted methylene moiety, and any M-M' moiety may be electronically saturated or unsaturated;

each occurrence of x is independently an integer from 1 - 6; and,

B<sup>2</sup>  
cont<sup>5</sup>

each occurrence of My is independently a methine group or a lower alkyl moiety which contains a methine group and optionally may be further substituted.

3. The compound of claim 2, wherein the phosphorus-containing moiety in R<sup>B</sup> is an aliphatic, heteroaliphatic, aryl, or heteroaryl group which comprises at least one of the substituents set forth in Series IIa:

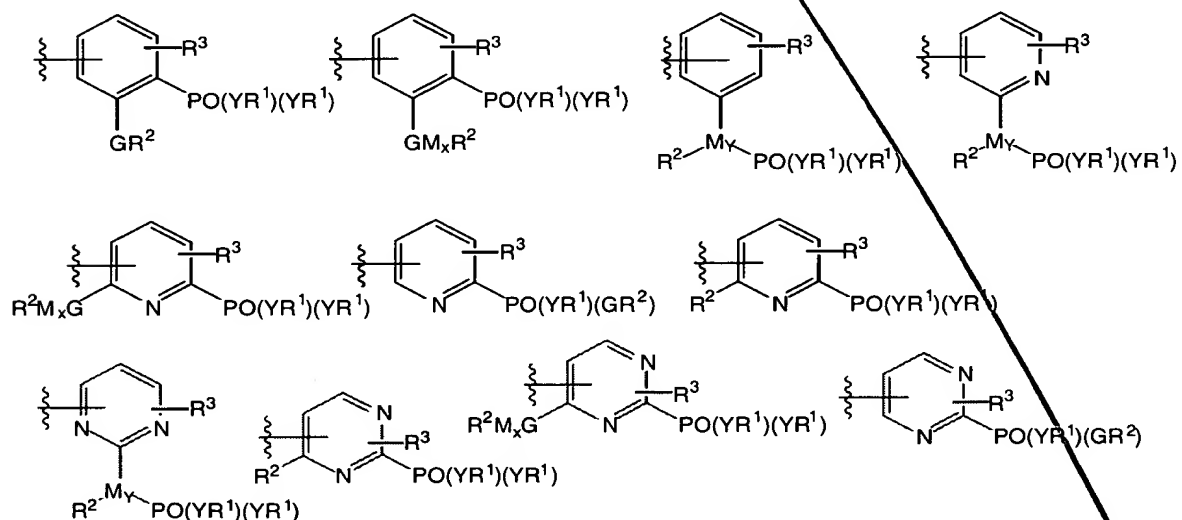


IIa

wherein each occurrence of R<sup>6</sup> is an independently selected aliphatic, heteroaliphatic, aryl, or heteroaryl moiety.

4. The compound of claim 3 in which R<sup>1</sup> is H or lower alkyl; M is -CH<sub>2</sub>-, -CH(OH)-, -CH(halo)-, or -C(halo)<sub>2</sub>-; R<sup>6</sup> is lower alkyl and R is H.

5. The compound of claim 1, wherein R<sup>B</sup> is any of the aryl or heteroaryl moieties of Series III:



III

B2  
cont

wherein each occurrence of Y is independently a covalent bond, -O-, -S- or -NR-;

each occurrence of R (without a further alphanumeric superscript) is independently hydrogen, or a substituted or unsubstituted aliphatic, heteroaliphatic, aryl, or heteroaryl moiety;

each occurrence of R<sup>1</sup> is independently a substituted or unsubstituted aliphatic, heteroaliphatic, aryl, or heteroaryl moiety, or, except in YR<sup>1</sup> moieties in which Y is a covalent bond, R<sup>1</sup> may also be H;

each occurrence of R<sup>2</sup> is independently R<sup>1</sup>, -PO(YR<sup>1</sup>)(YR<sup>1</sup>), -SO<sub>2</sub>(YR<sup>1</sup>) or -C(O)(YR<sup>1</sup>)

each occurrence of R<sup>3</sup> independently represents from 0-3 substituents independently selected from the group consisting of halogen; R, -GR, -CO(YR), acylamino, amido, amidino, cyano, nitro, azido, sulfonyl, sulfoxido, sulfate, sulfonate, sulfamoyl, sulfonamido, and substituents of Series II;

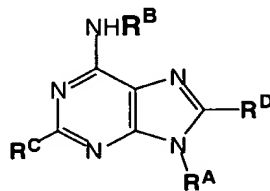
each occurrence of G is independently -O-, -S-, -NR- or M<sub>x</sub>;

each occurrence of M is independently a substituted or unsubstituted methylene moiety, and any M-M' moiety may be electronically saturated or unsaturated;

each occurrence of x is independently an integer from 1 - 6; and,

each occurrence of My is independently a methine group or a lower alkyl moiety which contains a methine group and optionally may be further substituted.

6. The compound of formula (I) (or a pharmaceutically acceptable derivative thereof):



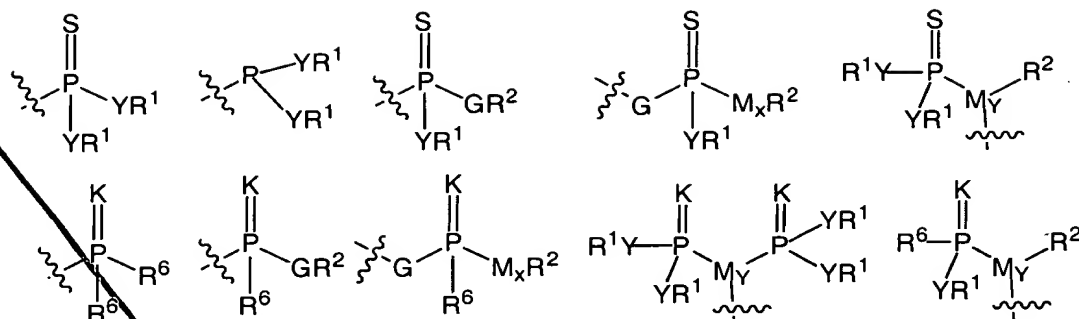
(I)

wherein

R<sup>A</sup> is hydrogen, or an aliphatic, heteroaliphatic, aryl, or heteroaryl moiety;

R<sup>B</sup> comprises an aliphatic, heteroaliphatic, aryl, or heteroaryl moiety bearing at least one a substituent of Series IIb:

B2  
cont



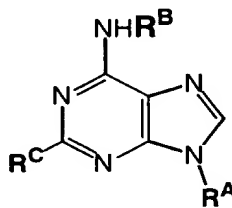
**IIb**

$R^C$  is hydrogen, halogen, an aliphatic, heteroaliphatic, aryl, or heteroaryl moiety, or  $-ZR$ ,  
 5 wherein  $Z$  is  $-O-$ ,  $-S-$ , or  $NR$ , wherein each occurrence of  $R$  without a further alphanumeric superscript is independently hydrogen, or a substituted or unsubstituted aliphatic, heteroaliphatic, aryl, or heteroaryl moiety;

$R^D$  is hydrogen, halogen, an aliphatic, heteroaliphatic, aryl, or heteroaryl moiety, or  $-ZR$ ;  
 wherein in each of the foregoing groups each aliphatic or heteroaliphatic moiety may be  
 10 branched or unbranched, cyclic or acyclic and substituted or unsubstituted, and each aryl and heteroaryl moiety may be substituted or unsubstituted;

with the proviso that (1)  $R^D$  is a moiety other than one comprising a substituted or unsubstituted arylene moiety (in which up to two methine carbons may be replaced by nitrogen atoms), a C3-7 cycloalkylene moiety (which may contain nitrogen atoms in place of up to two ring carbons), an indanylene moiety, or a 1,2,3,4-tetrahydronaphthylene moiety; or (2)  $R^D$  is a moiety  
 15 other than one terminating in a cyano group or in an N-substituted or unsubstituted amino, amidino, guanidino or guanidinoalkyl group.

7. The compound of formula (Ia) (or a pharmaceutically acceptable derivative thereof):



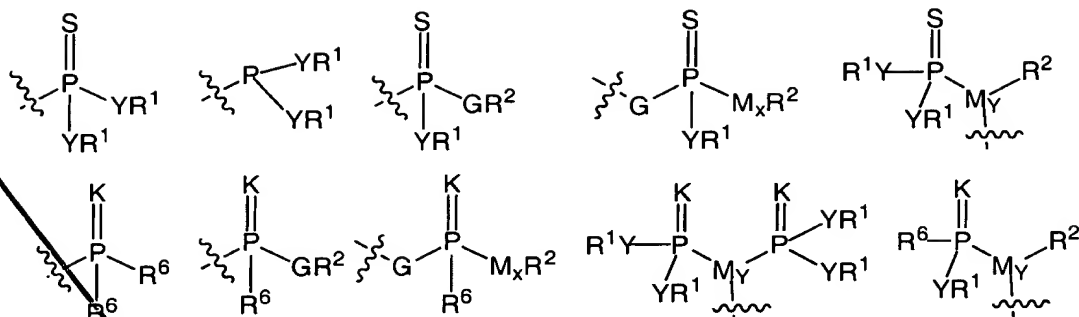
**(Ia)**

wherein

$R^A$  is hydrogen, or an aliphatic, heteroaliphatic, aryl, or heteroaryl moiety;

$R^B$  comprises an aliphatic, heteroaliphatic, aryl, or heteroaryl moiety bearing at least one a  
 25 substituent of Series IIb:

B<sup>2</sup>  
cont

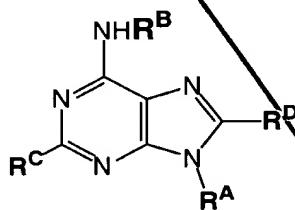


**IIb**

$R^C$  is hydrogen, halogen, an aliphatic, heteroaliphatic, aryl, or heteroaryl moiety, or  $-ZR$ ,  
 5 wherein  $Z$  is  $-O-$ ,  $-S-$ , or  $NR$ , wherein each occurrence of  $R$  without a further alphanumeric superscript is independently hydrogen, or a substituted or unsubstituted aliphatic, heteroaliphatic, aryl, or heteroaryl moiety; and,

$R^D$  is hydrogen, halogen, an aliphatic, heteroaliphatic, aryl, or heteroaryl moiety, or  $-ZR$ ;  
 wherein in each of the foregoing groups each aliphatic or heteroaliphatic moiety may be  
 10 branched or unbranched, cyclic or acyclic and substituted or unsubstituted, and each aryl and heteroaryl moiety may be substituted or unsubstituted.

8. The compound of formula (I) (or a pharmaceutically acceptable derivative thereof):



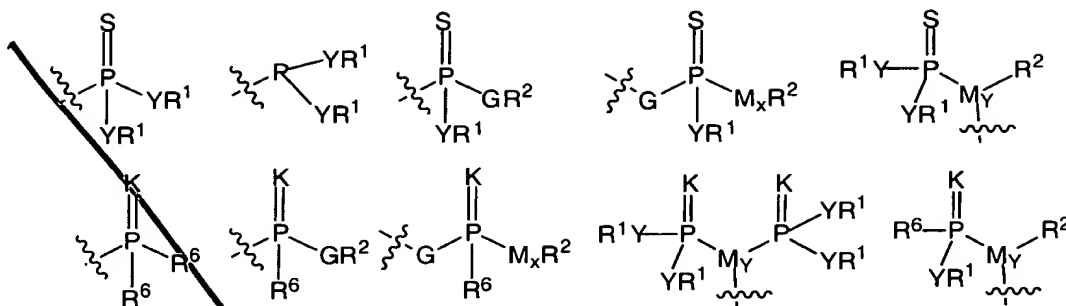
**(I)**

wherein

$R^A$  is hydrogen, or an aliphatic, heteroaliphatic, aryl, or heteroaryl moiety;

20  $R^B$  comprises an aliphatic, heteroaliphatic, aryl, or heteroaryl moiety bearing at least one a substituent of Series IIb:

B<sup>2</sup>  
cont

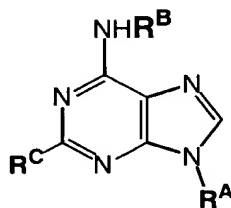


**IIb**

5  $R^C$  is hydrogen, halogen, an aliphatic, heteroaliphatic, aryl, or heteroaryl moiety, or -ZR, wherein Z is -O-, -S-, or NR, wherein each occurrence of R without a further alphanumeric superscript is independently hydrogen, or a substituted or unsubstituted aliphatic, heteroaliphatic, aryl, or heteroaryl moiety;

10  $R^D$  is hydrogen, halogen, or -YR, wherein R is a moiety which does not terminate in a cyano group or in an N-substituted or unsubstituted amino, amidino, guanidino or guanidinoalkyl group; wherein in each of the foregoing groups each aliphatic or heteroaliphatic moiety may be branched or unbranched, cyclic or acyclic and substituted or unsubstituted, and each aryl and heteroaryl moiety may be substituted or unsubstituted except as provided to the contrary.

15 9. The compound of formula (Ia) (or a pharmaceutically acceptable derivative thereof):



(Ia)

wherein

20  $R^A$  is hydrogen, or an aliphatic, heteroaliphatic, aryl, or heteroaryl moiety;

$R^B$  comprises an aliphatic, heteroaliphatic, aryl, or heteroaryl moiety bearing at least one a substituent of Series IIb:

[illegible]

5         $R^C$  is hydrogen, halogen, an aliphatic, heteroaliphatic, aryl, or heteroaryl moiety, or -ZR, wherein Z is -O-, -S-, or NR, wherein each occurrence of R without a further alphanumeric superscript is independently hydrogen, or a substituted or unsubstituted aliphatic, heteroaliphatic, aryl, or heteroaryl moiety;

10

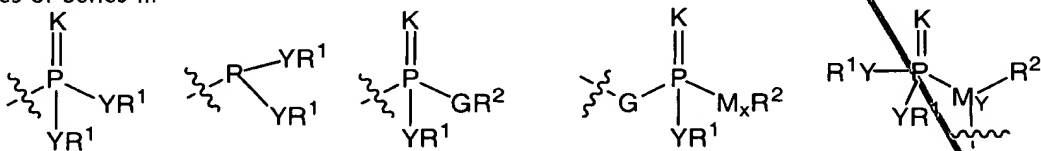
- 10.



15

$R^A$  is hydrogen, or an aliphatic, heteroaliphatic, aryl, or heteroaryl moiety;

$R^B$  is an aliphatic, heteroaliphatic, aryl, or heteroaryl moiety which comprises one or more of the moieties of Series II:

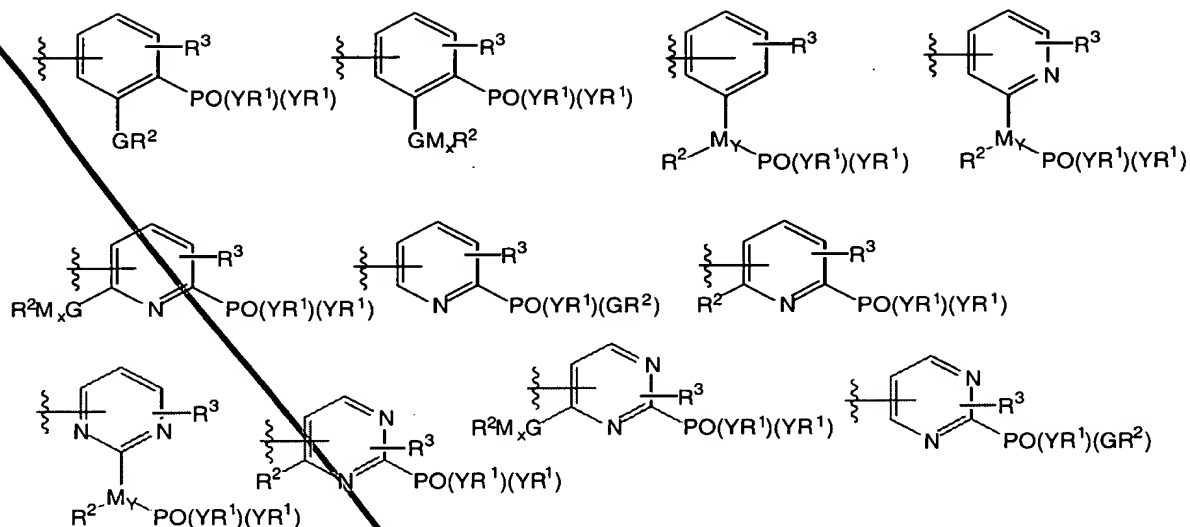


## 20

or is one of the moieties of Series III:



Pa  
cont



### III

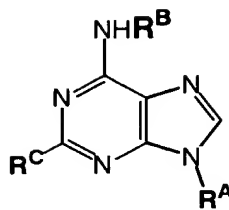
R<sup>C</sup> is hydrogen, halogen, an aliphatic, heteroaliphatic, aryl, or heteroaryl moiety, or -ZR, wherein Z is -O-, -S-, or NR, wherein each occurrence of R without a further alphanumeric superscript is independently hydrogen, or a substituted or unsubstituted aliphatic, heteroaliphatic, aryl, or heteroaryl moiety;

R<sup>D</sup> is hydrogen, halogen, or -YR, wherein R is a moiety which does not terminate in a cyano group or in an N-substituted or unsubstituted amino, amidino, guanidino or guanidinoalkyl group;

wherein in each of the foregoing groups each aliphatic or heteroaliphatic moiety may be branched or unbranched, cyclic or acyclic and substituted or unsubstituted, and each aryl and heteroaryl moiety may be substituted or unsubstituted;

with the proviso that (1) at least one of R<sup>A</sup>, R<sup>C</sup> or R<sup>D</sup> comprises a phosphorus-containing moiety; (2) R<sup>C</sup> is covalently attached through a C-C bond to the carbon atom at ring position 2 of the purine ring system; or (3) R<sup>B</sup> comprises a phosphorus-containing moiety other than -P(O)R<sup>J</sup>R<sup>J'</sup> where R<sup>J</sup> and R<sup>J'</sup> are independently OH, alkoxy, arylalkoxy, aryloxy, alkylcarbonyloxy-alkoxy, arylalkylcarbonyloxyalkoxy, NR<sup>k</sup>R<sup>k'</sup>, mono- or di-alkylaminocarbonylmethyloxy, (di-aryl-alkylaminocarbonylmethyloxy, arylamino, a D- or L- amino acid, N-alkyl)piperidine-4-yloxy, 2-methylsulfonylethoxy, 1,3 thiazole-2-ylmethyloxy, 3-pyridylmethyloxy, or 2-((di-alkyl)amino)ethoxy, where R<sup>k</sup> is H, alkyl, cycloalkyl, cycloalkylalkyl, or aryl or arylalkyl (1-5 carbon atoms of the aryl ring may be replaced with N, O or S), or R<sup>k</sup> and R<sup>k'</sup> together with the atoms that connect them form a ring system (which can also contain additional N, O or S atoms and which can be saturated or unsaturated).

11. The compound of formula (Ia) (or a pharmaceutically acceptable derivative thereof):

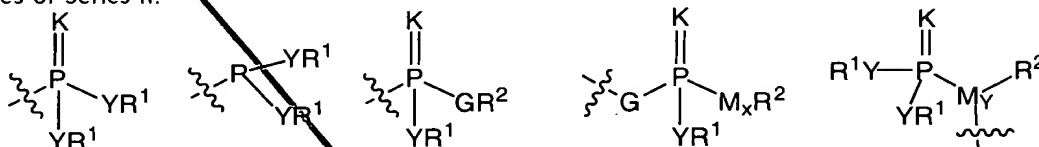


(Ia)

wherein

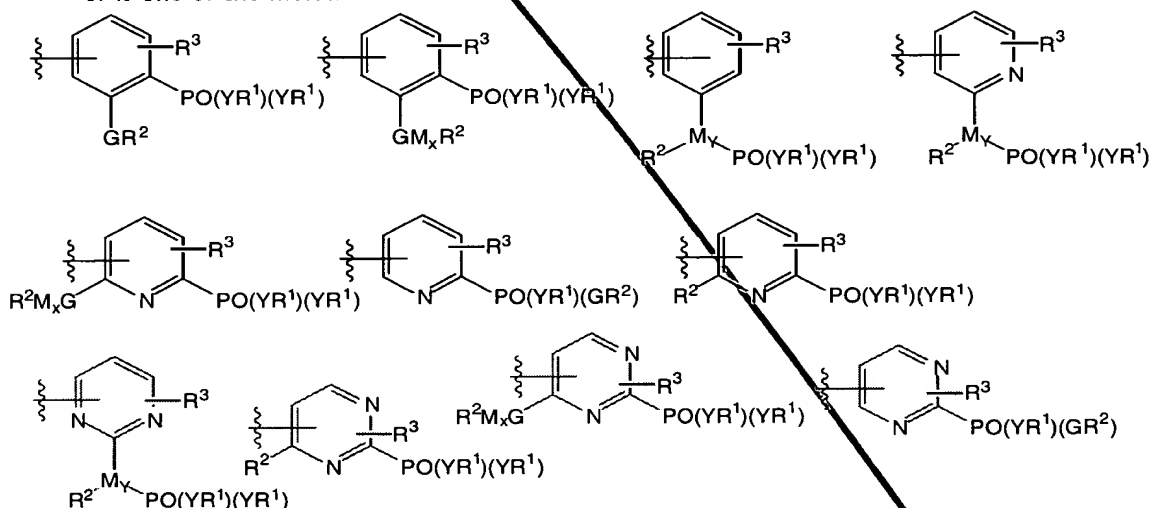
R<sup>A</sup> is hydrogen, or an aliphatic, heteroaliphatic, aryl, or heteroaryl moiety;

5 R<sup>B</sup> is an aliphatic, heteroaliphatic, aryl, or heteroaryl moiety which comprises one or more of the moieties of Series II:



II

or is one of the moieties of Series III:



III

10 R<sup>C</sup> is hydrogen, halogen, an aliphatic, heteroaliphatic, aryl, or heteroaryl moiety, or -ZR, wherein Z is -O-, -S-, or NR, wherein each occurrence of R without a further alphanumeric superscript is independently hydrogen, or a substituted or unsubstituted aliphatic, heteroaliphatic, aryl, or heteroaryl moiety; and,

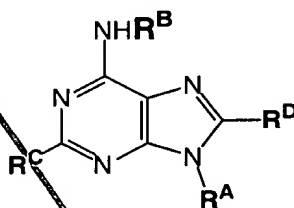
15 wherein in each of the foregoing groups each aliphatic or heteroaliphatic moiety may be branched or unbranched, cyclic or acyclic and substituted or unsubstituted, and each aryl and heteroaryl moiety may be substituted or unsubstituted;

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B2 cont

with the proviso that (1) at least one of  $R^A$  and  $R^C$  comprises a phosphorus-containing moiety; (2)  $R^C$  is covalently attached through a C-C bond to the carbon atom at ring position 2 of the purine ring system; or (3)  $R^B$  comprises a moiety other than  $-P(O)R^J R^{J'}$  where  $R^J$  and  $R^{J'}$  are independently OH, alkoxy, arylalkoxy, aryloxy, alkylcarbonyloxy-alkoxy, arylalkylcarbonyloxyalkoxy,  $NR^k R^{k'}$ , mono- or di-alkylaminocarbonylmethoxy, (di-aryl-alkylaminocarbonylmethoxy, arylamino, a D- or L- amino acid, N-alkyl)piperidine-4yloxy, 2-methylsulfonylethoxy, 1,3 thiazole-2-ylmethoxy, 3-pyridylmethoxy, or 2-((di-alkyl)amino)ethoxy, where  $R^k$  is H, alkyl, cycloalkyl, cycloalkylalkyl, or aryl or arylalkyl (1-5 carbon atoms of the aryl ring may be replaced with N, O or S), or  $R^k$  and  $R^{k'}$  together with the atoms that connect them form a ring system (which can also contain additional N, O or S atoms and which can be saturated or unsaturated).

12. The compound of formula (I) (or a pharmaceutically acceptable derivative thereof):



(I)

wherein

$R^A$  is hydrogen, or an aliphatic, heteroaliphatic, aryl, or heteroaryl moiety;

$R^B$  is an aliphatic, heteroaliphatic, aryl, or heteroaryl moiety which comprises one or more phosphorus-containing moieties;

$R^C$  is a branched, unbranched or cyclic alkyl group bearing one or more substituents; a branched, unbranched or cyclic alkoxy moiety substituted with one or more OR,  $NRR'$ , or substituted aryl moieties; a branched, unbranched or cyclic alkene or alkenoxy moiety which may be optionally substituted with one or more substituents; or  $NRR'$  where R and R' are independently selected from substituted or unsubstituted aliphatic and substituted aryl moieties;

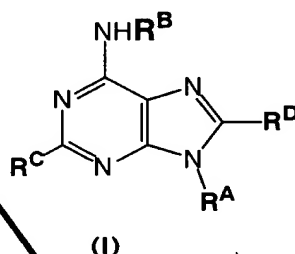
$R^D$  is hydrogen, halogen, or  $-YR$ , wherein R is a moiety which does not terminate in a cyano group or in an N-substituted or unsubstituted amino, amidino, guanidino or guanidinoalkyl group;

wherein in each of the foregoing groups each aliphatic or heteroaliphatic moiety may be branched or unbranched, cyclic or acyclic and substituted or unsubstituted, and each aryl and heteroaryl moiety may be substituted or unsubstituted;

with the proviso that (1) at least one of  $R^A$ ,  $R^C$  or  $R^D$  comprises a phosphorus-containing moiety; (2)  $R^C$  is covalently attached through a C-C bond to the carbon atom at ring position 2 of the purine ring system; or (3)  $R^B$  comprises a phosphorus-containing moiety other than  $-P(O)R^J R^{J'}$  where  $R^J$  and  $R^{J'}$  are independently OH, alkoxy, arylalkoxy, aryloxy, alkylcarbonyloxy-alkoxy,

B2  
cont 5  
arylalkylcarbonyloxyalkoxy,  $\text{NR}^k\text{R}^{k'}$ , mono- or di-alkylaminocarbonylmethoxy, (di-aryl-alkylaminocarbonylmethoxy, arylamino, a D- or L- amino acid, N-alkyl)piperidine-4yloxy, 2-methylsulfonylethoxy, 1,3 thiazole-2-ylmethoxy, 3-pyridylmethoxy, or 2-((di-alkyl)amino)ethoxy, where  $\text{R}^k$  is H, alkyl, cycloalkyl, cycloalkylalkyl, or aryl or arylalkyl (1-5 carbon atoms of the aryl ring may be replaced with N, O or S), or  $\text{R}^k$  and  $\text{R}^{k'}$  together with the atoms that connect them form a ring system (which can also contain additional N, O or S atoms and which can be saturated or unsaturated).

10 13. The compound of formula (I) (or a pharmaceutically acceptable derivative thereof):



wherein

15  $\text{R}^A$  is hydrogen; **halogen**; alkenyl; alkynyl; alkyl-; -alkylaryl where the aryl group contains at least one substituent,  $\text{R}^3$ ; -alkylheteroaryl which may be optionally substituted; or a substituted aryl or optionally substituted heteroaryl moiety;

$\text{R}^B$  is an aliphatic, heteroaliphatic, aryl, or heteroaryl moiety which comprises one or more phosphorus-containing moieties;

20  $\text{R}^C$  is hydrogen; halogen; an aliphatic, heteroaliphatic, aryl, or heteroaryl moiety; or -ZR, wherein Z is -O-, -S-, or NR, wherein each occurrence of R without a further alphanumeric superscript is independently hydrogen, or a substituted or unsubstituted aliphatic, heteroaliphatic, aryl, or heteroaryl moiety;

$\text{R}^D$  is hydrogen, halogen, or -YR, wherein R is a moiety which does not terminate in a cyano group or in an N-substituted or unsubstituted amino, amidino, guanidino or guanidinoalkyl group;

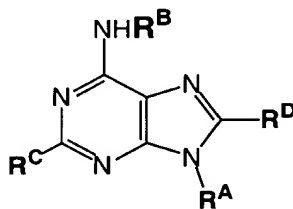
25 wherein in each of the foregoing groups each aliphatic or heteroaliphatic moiety may be branched or unbranched, cyclic or acyclic and substituted or unsubstituted, and each aryl and heteroaryl moiety may be substituted or unsubstituted;

30 with the proviso that (1) at least one of  $\text{R}^A$ ,  $\text{R}^C$  or  $\text{R}^D$  comprises a phosphorus-containing moiety; (2)  $\text{R}^C$  is covalently attached through a C-C bond to the carbon atom at ring position 2 of the purine ring system; or (3)  $\text{R}^B$  comprises a phosphorus-containing moiety other than  $-\text{P}(\text{O})\text{R}^J\text{R}^{J'}$  where  $\text{R}^J$  and  $\text{R}^{J'}$  are independently OH, alkoxy, arylalkoxy, aryloxy, alkylcarbonyloxy-alkoxy, arylalkylcarbonyloxyalkoxy,  $\text{NR}^k\text{R}^{k'}$ , mono- or di-alkylaminocarbonylmethoxy, (di-aryl-alkylaminocarbonylmethoxy, arylamino, a D- or L- amino acid, N-alkyl)piperidine-4yloxy, 2-

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B2  
cont

methysulfonylethoxy, 1,3 thiazole-2-ylmethoxy, 3-pyridylmethoxy, or 2-((di-alkyl)amino)ethoxy, where  $R^k$  is H, alkyl, cycloalkyl, cycloalkylalkyl, or aryl or arylalkyl (1-5 carbon atoms of the aryl ring may be replaced with N, O or S), or  $R^k$  and  $R^{k'}$  together with the atoms that connect them form a ring system (which can also contain additional N, O or S atoms and which can be saturated or unsaturated).

14. The compound of formula (I) (or a pharmaceutically acceptable derivative thereof):



(I)

wherein

$R^A$  is hydrogen, or an aliphatic, heteroaliphatic, aryl, or heteroaryl moiety;

$R^B$  is an aliphatic, heteroaliphatic, aryl, or heteroaryl moiety which comprises one or more phosphorus-containing moieties;

$R^C$  is hydrogen, halogen, an aliphatic, heteroaliphatic, aryl, or heteroaryl moiety, or -ZR, wherein Z is -O-, -S-, or NR, wherein each occurrence of R without a further alphanumeric superscript is independently hydrogen, or a substituted or unsubstituted aliphatic, heteroaliphatic, aryl, or heteroaryl moiety;

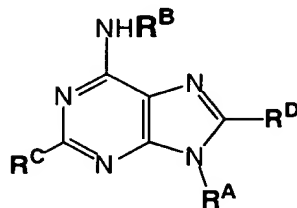
$R^D$  is hydrogen, halogen, or -YR, wherein R is a moiety which does not terminate in a cyano group or in an N-substituted or unsubstituted amino, amidino, guanidino or guanidinoalkyl group;

at least one of  $R^A$ ,  $R^B$  and  $R^C$  also contains an independently selected phosphorus-containing moiety;

wherein in each of the foregoing groups each aliphatic or heteroaliphatic moiety may be branched or unbranched, cyclic or acyclic and substituted or unsubstituted, and each aryl and heteroaryl moiety may be substituted or unsubstituted;

with the proviso that in compounds in which  $R^C$  is H, OH, halogen, alkoxy or cycloalkoxy groups of 1 to 6 carbon atoms (which alkoxy and cycloalkoxy groups can be substituted with phenyl) or amine, which can be substituted with phenyl or with alkyl or cycloalkyl groups of 1 to 6 carbon atoms, and  $R^A$  is benzyl, phenyl or C1-4 alkyl, optionally substituted with oxygen (e.g. in the form of an ether or alcohol),  $R^B$  is a moiety other than a heteroatom- and halogen-substituted derivative of a 3 to 8 carbon cycloalkyl, a 1 to 10 carbon alkyl, a 6 to 13 carbon aryl, or a 7 to 14 carbon aralkyl moiety in which the heteroatom is selected from N, P, S and O

15. The compound of formula (I) (or a pharmaceutically acceptable derivative thereof):

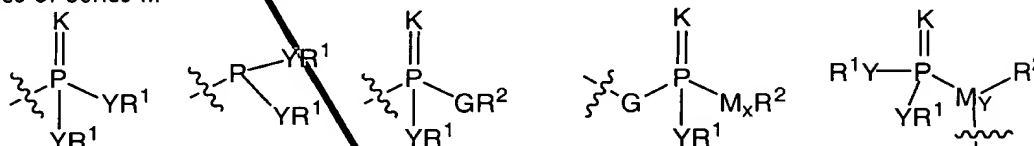


(I)

wherein

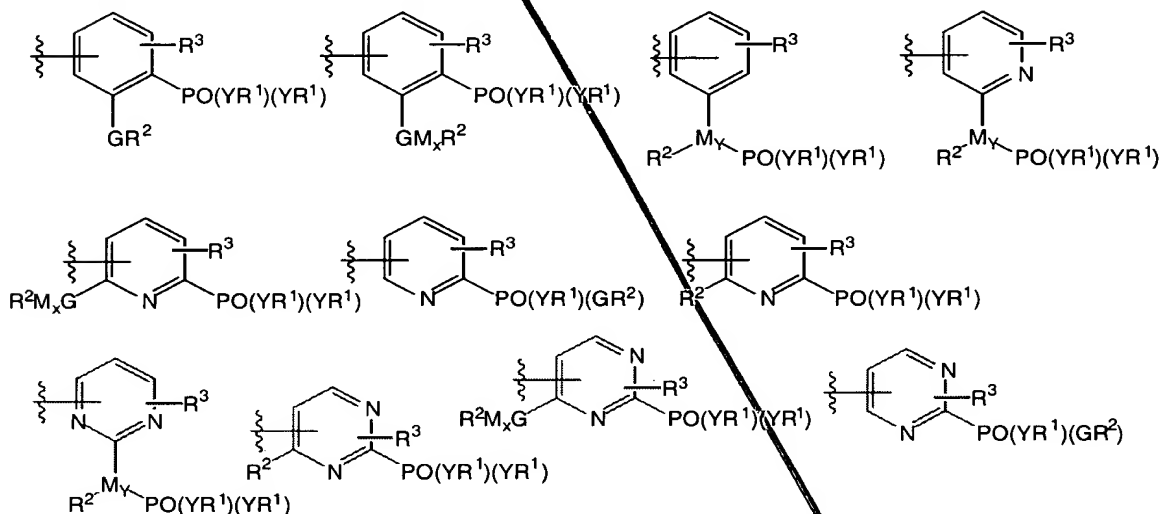
$R^A$  is hydrogen, or an aliphatic, heteroaliphatic, aryl, or heteroaryl moiety;

$R^B$  is an aliphatic, heteroaliphatic, aryl, or heteroaryl moiety which comprises one or more of the moieties of Series II:



II

or is one of the moieties of Series III:



III

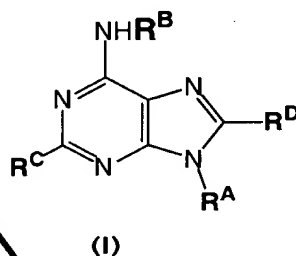
$R^C$  is hydrogen, halogen, an aliphatic, heteroaliphatic, aryl, or heteroaryl moiety, or -ZR, wherein Z is -O-, -S-, or NR, wherein each occurrence of R without a further alphanumeric superscript is independently hydrogen, or a substituted or unsubstituted aliphatic, heteroaliphatic, aryl, or heteroaryl moiety;

$R^D$  is hydrogen, halogen, or -YR, wherein R is a moiety which does not terminate in a cyano group or in an N-substituted or unsubstituted amino, amidino, guanidino or guanidinoalkyl group;

B<sup>a</sup>  
cont  
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at least one of R<sup>A</sup>, R<sup>B</sup> and R<sup>C</sup> also contains an independently selected phosphorus-containing moiety;  
wherein in each of the foregoing groups each aliphatic or heteroaliphatic moiety may be branched or unbranched, cyclic or acyclic and substituted or unsubstituted, and each aryl and heteroaryl moiety may be substituted or unsubstituted.

16. The compound of formula (I) (or a pharmaceutically acceptable derivative thereof):



wherein

R<sup>A</sup> is hydrogen, or an aliphatic, heteroaliphatic, aryl, or heteroaryl moiety;

R<sup>B</sup> is an aliphatic, heteroaliphatic, aryl, or heteroaryl moiety which comprises one or more phosphorus-containing moieties;

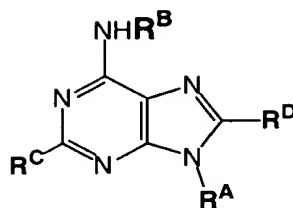
R<sup>C</sup> is a branched, unbranched or cyclic alkyl group bearing one or more substituents; a branched, unbranched or cyclic alkoxy moiety substituted with one or more OR, NRR', or substituted aryl moieties; a branched, unbranched or cyclic alkene or alkenoxy moiety which may be optionally substituted with one or more substituents; or NRR' where R and R' are independently selected from substituted or unsubstituted aliphatic and substituted aryl moieties;

R<sup>D</sup> is hydrogen, halogen, or -YR, wherein R is a moiety which does not terminate in a cyano group or in an N-substituted or unsubstituted amino, amidino, guanidino or guanidinoalkyl group;

at least one of R<sup>A</sup>, R<sup>B</sup> and R<sup>C</sup> also contains an independently selected phosphorus-containing moiety;

wherein in each of the foregoing groups each aliphatic or heteroaliphatic moiety may be branched or unbranched, cyclic or acyclic and substituted or unsubstituted, and each aryl and heteroaryl moiety may be substituted or unsubstituted.

17. The compound of formula (I) (or a pharmaceutically acceptable derivative thereof):



(I)

wherein

R<sup>A</sup> is hydrogen; **halogen**; alkenyl; alkynyl; alkyl- or alkenyl-aryl where the aryl group contains at least one substituent, R<sup>3</sup>; or a substituted aryl or heteroaryl moiety; R<sup>B</sup> is an aliphatic, heteroaliphatic, aryl, or heteroaryl moiety which comprises one or more phosphorus-containing moieties;

R<sup>C</sup> is hydrogen, halogen, an aliphatic, heteroaliphatic, aryl, or heteroaryl moiety, or -ZR, wherein Z is -O-, -S-, or NR, wherein each occurrence of R without a further alphanumeric superscript is independently hydrogen, or a substituted or unsubstituted aliphatic, heteroaliphatic, aryl, or heteroaryl moiety;

R<sup>D</sup> is hydrogen, halogen, or -YR, wherein R is a moiety which does not terminate in a cyano group or in an N-substituted or unsubstituted amino, amidino, guanidino or guanidinoalkyl group;

at least one of R<sup>A</sup>, R<sup>B</sup> and R<sup>C</sup> also contains an independently selected phosphorus-containing moiety;

wherein in each of the foregoing groups each aliphatic or heteroaliphatic moiety may be branched or unbranched, cyclic or acyclic and substituted or unsubstituted, and each aryl and heteroaryl moiety may be substituted or unsubstituted;

18. The compound of any of of claims 1 to 17 in which R<sup>D</sup> is H or halo.

19. The compound of any of of claims 1 to 18 in which the phosphorus-containing moiety of R<sup>B</sup> is present on an aryl or heteroaryl ring system.

20. The compound of any of of claims 1 to 19 in which R<sup>A</sup> is lower aliphatic, and may be branched or unbranched, cyclic or acyclic, and optionally substituted with one or more substituents selected from a lower aliphatic group (which may be substituted or unsubstituted), -OR, -SR, -NRR', -C(O)YR, and -Y-C(O)Y'R, where Y is O, S, NR, or a bond and R is H or a substituted or unsubstituted aliphatic, heteroaliphatic, aryl, or heteroaryl moiety.

21. The compound of claim 20 in which R<sup>A</sup> is lower aliphatic which may be substituted with one or more hydroxy, alkoxy, aralkoxy, carbamyl, amino, substituted amino, acyl, cyano, halogen, nitro or sulfo groups, and/or with one or more alkyl, alkenyl, alkynyl, cycloalkyl, aryl, heterocyclic, aryloxy or aralkyl moieties which may themselves be substituted with one or more hydroxy, alkoxy, aralkoxy, carbamyl, amino, substituted amino, acyl, cyano, halogen, nitro or sulfo groups.



B<sup>2</sup>  
cont

22. The compound of claim 20 in which R<sup>A</sup> is Mx-aryl or Mx-heterocycle where M is a substituted or unsubstituted methylene, x is an integer from 1 to 6, the aryl moiety may bear one or more substituents, and the heterocycle is a substituted or unsubstituted, aromatic or nonaromatic heterocyclic moiety comprising a 5- to 7-membered ring bearing one or more heteroatoms.

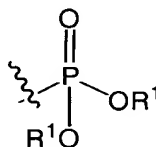
23. The compound of claim 21 wherein M<sub>x</sub> is methylene, ethylene or propylene, and the aryl moiety is o-, m-, or p-hydroxy-, 2,3-dihydroxy-, 2,4-dihydroxy-, 2,5-dihydroxy-, 3,4-dihydroxy-, or 3,5-dihydroxyphenyl.

24. The compound of any of claims 1 to 23, wherein R<sup>C</sup> is -OR, where R is H, aliphatic, heteroaliphatic, aryl, or heteroaryl.

25. The compound of any of claims 1 to 23, wherein R<sup>C</sup> is -R, -NR or -OR in which R is C1-C8 aliphatic, which may be branched or unbranched, cyclic or noncyclic, and which may be substituted with one or more hydroxy, alkoxy, aralkoxy, carbamyl, amino, substituted amino, acyl, cyano, halogen, nitro or sulfo groups, and/or with one or more alkyl, alkenyl, alkynyl, cycloalkyl, aryl, heterocyclic, aryloxy or aralkyl moieties which may themselves be substituted with one or more hydroxy, alkoxy, aralkoxy, carbamyl, amino, substituted amino, acyl, cyano, halogen, nitro or sulfo groups.

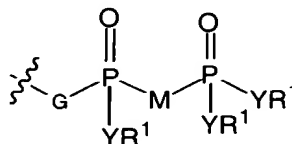
26. The compound of any of claims 1 to 23, wherein R comprises a C1-C8 aliphatic moiety substituted with one or more groups selected from the following: a substituted or unsubstituted amine or 5- to 7-membered heterocyclic moiety, which may itself be optionally substituted.

27. The compound of any of claims 1 to 26 in which R<sup>B</sup> comprises



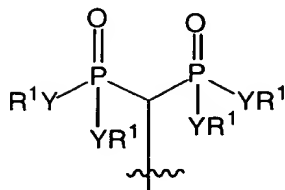
wherein each R<sup>1</sup> is independently H, alkyl, arylalkyl, aryl or a prodrug moiety.

28. The compound of any of claims 1 to 26 in which R<sup>B</sup> comprises



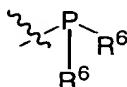
wherein each R<sup>1</sup> is independently H, alkyl, arylalkyl, aryl or a prodrug moiety.

29. The compound of any of claims 1 to 26 in which R<sup>B</sup> comprises



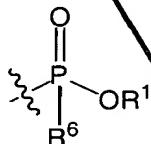
wherein each R<sup>1</sup> is independently H, alkyl, arylalkyl, aryl or a prodrug moiety.

30. The compound of any of claims 1 to 26 in which R<sup>B</sup> comprises



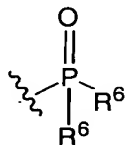
wherein each R<sup>6</sup> is independently alkyl, arylalkyl, aryl or a prodrug moiety.

31. The compound of any of claims 1 to 26 in which R<sup>B</sup> comprises



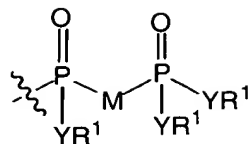
wherein R<sup>1</sup> is H, alkyl, arylalkyl or a prodrug moiety and R<sup>6</sup> is aliphatic, heteroaliphatic, aryl, or heteroaryl or a prodrug moiety.

32. The compound of any of claims 1 to 26 in which R<sup>B</sup> comprises



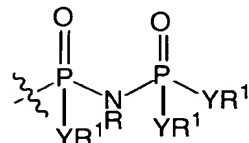
wherein each R<sup>6</sup> is independently aliphatic, heteroaliphatic, aryl, or heteroaryl or a prodrug moiety.

33. The compound of any of claims 1 to 26 in which R<sup>B</sup> comprises



wherein each R<sup>1</sup> is H, alkyl, arylalkyl or a prodrug moiety, and Y and M are as defined previously.

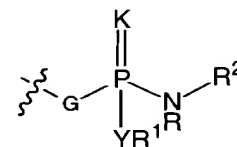
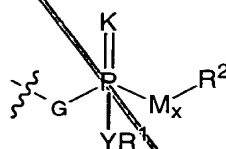
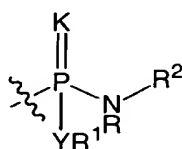
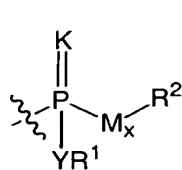
- 5 34. The compound of any of claims 1 to 26 in which R<sup>B</sup> comprises



wherein each R<sup>1</sup> is independently H, alkyl, arylalkyl, aryl or a prodrug moiety and R is aliphatic, heteroaliphatic, aryl, or heteroaryl.

10

35. The compound of any of claims 3, 6, 7, 8 or 9 in which R<sup>B</sup> comprises one of the following structures



15

in place of a substituent of Series IIa or IIb,

wherein each occurrence of each of the following is as indicated:

G is O, S, NR or M<sub>x</sub>;

K is O or S;

20 Y is O, S, NR or a chemical bond linking R<sup>1</sup> to P;

R<sup>1</sup> is H, alkyl, arylalkyl or a prodrug moiety;

M is substituted or unsubstituted methylene;

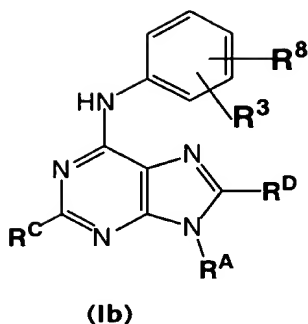
x is an integer from 1 to 6; and,

R<sup>2</sup> is R<sup>1</sup>, PK(YR<sup>1</sup>)(YR<sup>1</sup>), -SO<sub>2</sub>(YR<sup>1</sup>) or -C(O)(YR<sup>1</sup>).

25

36. A compound of formula (Ib) (or a pharmaceutically acceptable derivative thereof):

B2  
cont



wherein

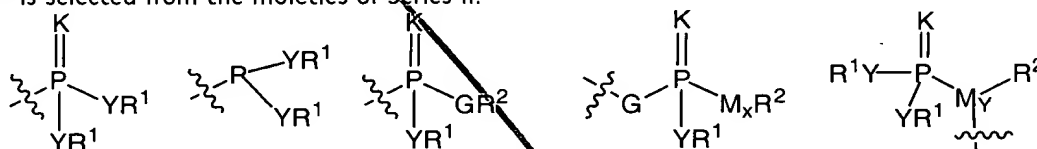
$R^A$  is hydrogen, or an aliphatic, heteroaliphatic, aryl, or heteroaryl moiety;

5  $R^C$  is hydrogen, halogen, an aliphatic, heteroaliphatic, aryl, or heteroaryl moiety, or  $-ZR$ ,

wherein Z is  $-O-$ ,  $-S-$ , or  $NR$ , wherein each occurrence of R without a further alphanumeric superscript is independently hydrogen, or a substituted or unsubstituted aliphatic, heteroaliphatic, aryl, or heteroaryl moiety;

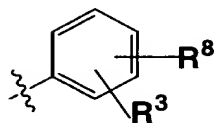
$R^D$  is hydrogen, halogen, an aliphatic, heteroaliphatic, aryl, or heteroaryl moiety, or  $-ZR$ ;

10  $R^8$  is selected from the moieties of Series II:



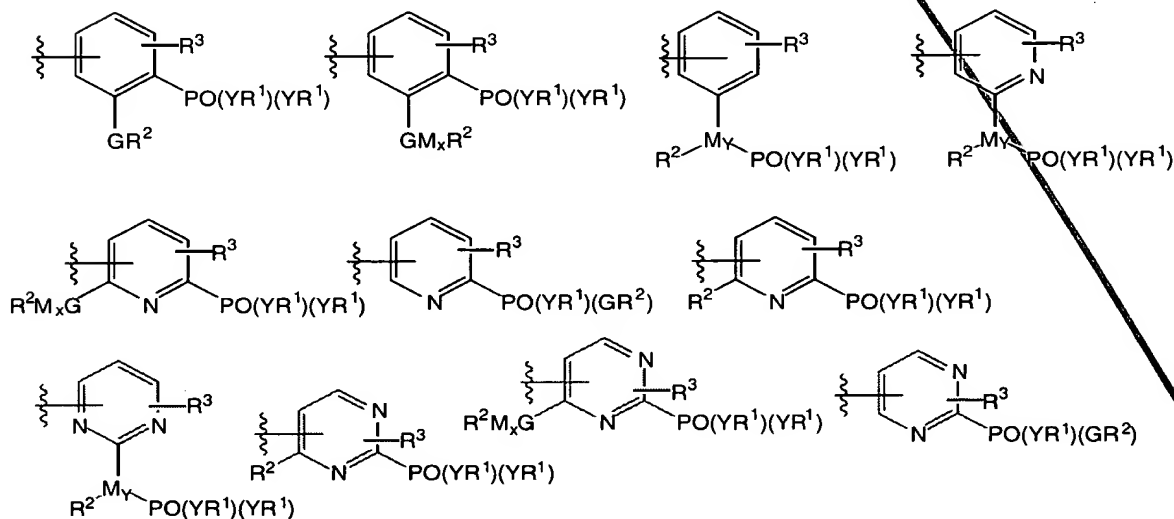
II

or



15

is selected from the moieties of Series III:



III

*B2 cont*<sup>5</sup>  
R<sup>3</sup> represents from 0-3 substituents independently selected from the group consisting of halogen; R, -GR, -CO(YR), acylamino, amido, amidino, cyano, nitro, azido, sulfonyl, sulfoxido, sulfate, sulfonate, sulfamoyl, sulfonamido, and substituents of Series II;

wherein in each of the foregoing groups each aliphatic or heteroaliphatic moiety may be branched or unbranched, cyclic or acyclic and substituted or unsubstituted, and each aryl and heteroaryl moiety may be substituted or unsubstituted;

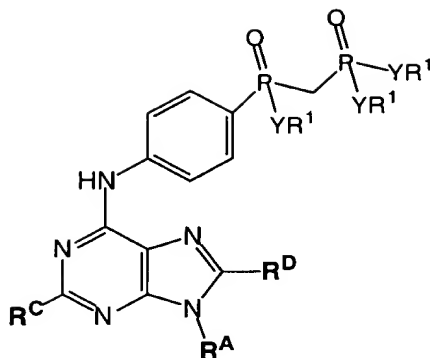
with the following provisos:

10 (A) (1) R<sup>D</sup> is a moiety other than one comprising a substituted or unsubstituted arylene moiety (in which up to two methine carbons may be replaced by nitrogen atoms), a C3-7 cycloalkylene moiety (which may contain nitrogen atoms in place of up to two ring carbons), an indanylene moiety, or a 1,2,3,4-tetrahydronaphthylene moiety; or (2) R<sup>D</sup> is a moiety other than one terminating in a cyano group or in an N-substituted or unsubstituted amino, amidino, guanidino or guanidinoalkyl group;

15 (B) in compounds in which R<sup>C</sup> is H, OH, halogen, alkoxy or cycloalkoxy groups of 1 to 6 carbon atoms (which alkoxy and cycloalkoxy groups can be substituted with phenyl) or amine, which can be substituted with phenyl or with alkyl or cycloalkyl groups of 1 to 6 carbon atoms, and R<sup>A</sup> is benzyl, 20 phenyl or C1-4 alkyl, optionally substituted with oxygen (e.g. in the form of an ether or alcohol), R<sup>B</sup> is a moiety other than a heteroatom- and halogen-substituted derivative of a 3 to 8 carbon cycloalkyl, a 1 to 10 carbon alkyl, a 6 to 13 carbon aryl, or a 7 to 14 carbon aralkyl moiety in which the heteroatom is selected from N, P, S and O; and,

25 (C) (1) at least one of R<sup>A</sup>, R<sup>C</sup> or R<sup>D</sup> comprises a phosphorus-containing moiety; (2) R<sup>C</sup> is covalently attached through a C-C bond to the carbon atom at ring position 2 of the purine ring system; or (3) R<sup>B</sup> comprises a phosphorus-containing moiety other than -P(O)R<sup>J</sup>R<sup>J'</sup> where R<sup>J</sup> and R<sup>J'</sup> are independently OH, alkoxy, arylalkoxy, aryloxy, alkylcarbonyloxy-alkoxy, arylalkylcarbonyloxyalkoxy, NR<sup>k</sup>R<sup>k'</sup>, mono- or 30 di-alkylaminocarbonylmethyloxy, (di-aryl-alkylaminocarbonylmethyloxy, arylamino, a D- or L- amino acid, N-alkyl)piperidine-4yloxy, 2-methylsulfonylethoxy, 1,3 thiazole-2-ylmethyloxy, 3-pyridylmethyloxy, or 2-((di-alkyl)amino)ethoxy, where R<sup>k</sup> is H, alkyl, cycloalkyl, cycloalkylalkyl, or aryl or arylalkyl (1-5 carbon atoms of the aryl ring may be replaced with N, O or S), or R<sup>k</sup> and R<sup>k'</sup> together with the atoms that connect them form a ring system (which can also contain additional N, O or S atoms and which can be saturated or unsaturated).

35  
37. The compound (or a pharmaceutically acceptable derivative thereof) of the formula :



wherein

$R^A$  is hydrogen, or an aliphatic, heteroaliphatic, aryl, or heteroaryl moiety;

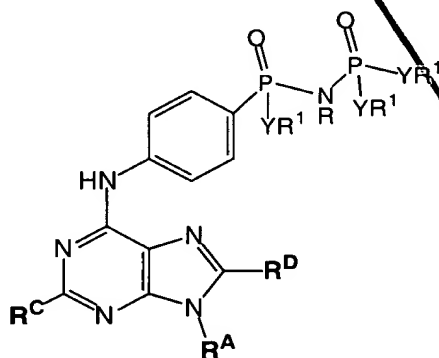
5  $R^C$  is hydrogen, halogen, an aliphatic, heteroaliphatic, aryl, or heteroaryl moiety, or -ZR, wherein Z is -O-, -S-, or NR, wherein each occurrence of R without a further alphanumeric superscript is independently hydrogen, or a substituted or unsubstituted aliphatic, heteroaliphatic, aryl, or heteroaryl moiety;

10  $R^D$  is hydrogen, halogen, an aliphatic, heteroaliphatic, aryl, or heteroaryl moiety, or -ZR, with the proviso that  $R^D$  does not terminate in a cyano group or in an N-substituted or unsubstituted amino, amidino, guanidino or guanidinoalkyl group; and

wherein in each of the foregoing groups each aliphatic or heteroaliphatic moiety may be branched or unbranched, cyclic or acyclic and substituted or unsubstituted, and each aryl and heteroaryl moiety may be substituted or unsubstituted.

15

38. The compound (or a pharmaceutically acceptable derivative thereof) of the formula :



(I)

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wherein

$R^A$  is hydrogen, or an aliphatic, heteroaliphatic, aryl, or heteroaryl moiety;

$R^C$  is hydrogen, halogen, an aliphatic, heteroaliphatic, aryl, or heteroaryl moiety, or -ZR, wherein Z is -O-, -S-, or NR, wherein each occurrence of R without a further alphanumeric superscript is

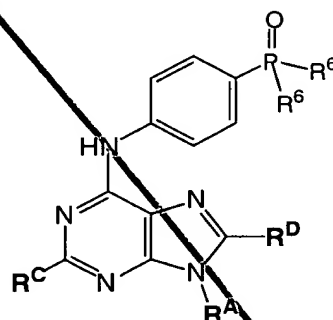
B<sup>2</sup>  
cont  
5 independently hydrogen, or a substituted or unsubstituted aliphatic, heteroaliphatic, aryl, or heteroaryl moiety;

R<sup>D</sup> is hydrogen, halogen, an aliphatic, heteroaliphatic, aryl, or heteroaryl moiety, or -ZR, with the proviso that R<sup>D</sup> does not terminate in a cyano group or in an N-substituted or unsubstituted amino, amidino, guanidino or guanidinoalkyl group; and

wherein in each of the foregoing groups each aliphatic or heteroaliphatic moiety may be branched or unbranched, cyclic or acyclic and substituted or unsubstituted, and each aryl and heteroaryl moiety may be substituted or unsubstituted.

10

39. The compound (or a pharmaceutically acceptable derivative thereof) of the formula :



15

wherein

R<sup>A</sup> is hydrogen, or an aliphatic, heteroaliphatic, aryl, or heteroaryl moiety;

R<sup>C</sup> is hydrogen, halogen, an aliphatic, heteroaliphatic, aryl, or heteroaryl moiety, or -ZR,

wherein Z is -O-, -S-, or NR, wherein each occurrence of R without a further alphanumeric superscript is independently hydrogen, or a substituted or unsubstituted aliphatic, heteroaliphatic, aryl, or heteroaryl moiety;

20

R<sup>D</sup> is hydrogen, halogen, an aliphatic, heteroaliphatic, aryl, or heteroaryl moiety, or -ZR, with the proviso that R<sup>D</sup> does not terminate in a cyano group or in an N-substituted or unsubstituted amino, amidino, guanidino or guanidinoalkyl group; and

wherein in each of the foregoing groups each aliphatic or heteroaliphatic moiety may be branched or

25

unbranched, cyclic or acyclic and substituted or unsubstituted, and each aryl and heteroaryl moiety may be substituted or unsubstituted.

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40. A composition containing a compound of any of claims 1 to 39 and one or more pharmaceutically acceptable excipient or additive.

B2  
cont  
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41. A pharmaceutical preparation comprising at least one compound of any of claims 1 to 39 or a pharmaceutically acceptable derivative thereof, as inhibitors of bone resorption by osteoclasts, as inhibitors of tumor growth and tumor metastasis, for the treatment and prophylaxis of diseases or undesirable conditions which are mediated by a kinase inhibited by said compound, and at least one pharmaceutically acceptable excipient or additive.

42. A pharmaceutical preparation comprising at least one compound of any of claims 1 to 39 or a pharmaceutically acceptable derivative thereof, and at least one pharmaceutically innocuous excipient or additive.

43. A method for inhibiting bone resorptions, inhibiting tumor growth and/or tumor metastasis, or for the treatment and prevention of diseases or undesirable conditions which are mediated by a kinase inhibited by compound of any of claims 1 to 39, comprising administering a therapeutically effective amount of said compound or a pharmaceutically acceptable derivative thereof to a human or animal in need thereof.

44. A method for inhibiting bone resorption by osteoclasts, comprising administering a therapeutically effective amount of a compound of any of claims 1 to 39, or a pharmaceutically acceptable derivative thereof, to a human or animal in need thereof.

45. A method for inhibiting tumor growth and/or tumor metastasis, comprising administering a therapeutically effective amount of a compound of any of claims 1 to 39, or a pharmaceutically acceptable derivative thereof, to a human or animal in need thereof.

46. A method for the treatment and prophylaxis of diseases which are mediated by a kinase inhibited by a compound of any of claims 1 to 39, comprising administering a therapeutically effective amount of said compound, or a pharmaceutically acceptable derivative thereof, to a human or animal in need thereof.